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Bound electron pairs in strongly correlated models of high-temperature superconductivity

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The ground-state energy of two electrons on a ring is calculated for the one-dimensional Hubbard model with positive and negative on-site interaction and for the contraction model with additive and multiplicative interaction terms. The $hc/2e$ periodicity of the ground-state energy with respect to a flux Φ threading the loop is derived. The periodicity may serve as an indication of superconductivity. The results are shown to be consistent with the Lieb–Wu solution for $\Phi=0$ limit. In addition, the new states that were missing in the Lieb–Wu solution are derived. © *1998 American Institute of Physics.* [S1063-777X(98)00504-0]

1. INTRODUCTION

Among the possible mechanisms of high temperature superconductivity attention was focused in the last years on strongly correlated systems,[1] non Fermi-liquid scenarios,[2,3] magnetic schemes (spin-fluctuation[4,5] and spin-bag[6]) and soft orbital mode interaction mechanisms.[7,8] The generic Hamiltonian underlying these models are the one-, two-, or three-band Hubbard positive- or negative-U Hamiltonians and contraction Hamiltonians with a hopping amplitude which depends upon the sum or product of the near-site occupation number operators. The criterion for superconductivity can be learned in the pairing instability, in the Meissner effect, or in flux quantization. In this paper some of the above models are considered in an assumption that halving of the flux periodicity in the energy versus flux dependence (hc/e to $hc/2e$) may serve as an indication of the superconducting transition.

The purpose of this paper is to show some new states for the one-dimensional Hubbard model, which are missing in the Lieb–Wu[9] solution, and to show that the contraction model may serve as a mechanism for superconductivity. Similar states appear in other strongly correlated models of high-T_c superconductivity. Specifically, we will analyze in this paper three Hamiltonians for strongly correlated fermions:

(1) Hubbard model with repulsive on-site interaction.[5]
(2) Negative-U Hubbard Hamiltonians.[27,28]
(3) Contraction-pairing mechanisms.[7,8,10]

It is known that direct O-O hopping in high-T_c superconductors is important. Since oxygen in oxides like $YBa_2Cu_3O_{6+x}$ has almost filled p-shell configuration, holes in a p^6 shell may play a similar role for the conduction in oxides in question, as the electrons from nearly empty atomic shells in conventional metals do. Oxygen atoms are specific in the sense that change of the oxygen ionization state (O^0 to O^- and O^{2-}) results in a dramatic increase of p_x, p_y orbitals in the CuO plane, and therefore in the increase of the magnitude of hopping between near oxygen (as well as near oxygen-copper) sites. A non-s-wave orbital configuration[10] is expected to survive with consideration of this occupation-dependent hopping.

2. GROUND-STATE ENERGY OF TWO ELECTRONS IN THE HUBBARD MODEL WITH POSITIVE AND NEGATIVE ON-SITE INTERACTION

We consider a loop of N_a lattice sites with a magnetic flux Φ threading the loop (Fig. 1). The electrons can hop between neighboring lattice sites, and each site can be occupied by at most two electrons with opposite spins. The Hamiltonian for this system has the form

$$H=-t\sum_{j,\sigma}\left(c^+_{j,\sigma}c_{j+1,\sigma}e^{i\alpha}+c^+_{j+1,\sigma}c_{j,\sigma}e^{-i\alpha}\right)+U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{1}$$

where $c^+_{j,\sigma}$ and $c_{j\sigma}$ are respectively the creation and annihilation operators of an electron with spin projection σ at the jth lattice site, t is the electron hopping amplitude, $\alpha=(2\pi/N_a)(\Phi/\Phi_0)$ (here $\Phi_0=hc/e$ is the magnetic flux quantum), $n_{j\sigma}$ is the occupation number operator, and U is on-site interaction term. The energy spectrum of H is invariant under the replacement of t by $-t$. Hence, we assume $t=+1$ in appropriate units.

The wave function for two electrons, one with spin up and the other with spin down, is

$$|\Psi\rangle=\sum_{x_1,x_2} f(x_1,x_2)c^+_{x_1\downarrow}c^+_{x_2\uparrow}|0\rangle, \tag{2}$$

where $|0\rangle$ is a vacuum state.

The eigenvalue equation $H|\Psi\rangle=E|\Psi\rangle$ leads to

$$-[(f(x_1+1,x_2)+f(x_1,x_2+1))e^{i\alpha}+(f(x_1-1,x_2)+f(x_1,x_2-1))e^{-i\alpha}]+U\delta(x_1,x_2)f(x_1,x_2)=Ef(x_1,x_2) \tag{3}$$

or, in the momentum space,

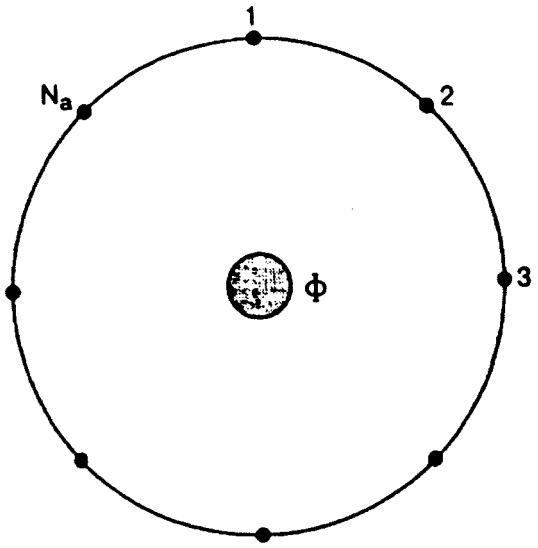

FIG. 1. Configuration of the sample. There are N_a lattice sites on the ring which can be numbered from 1 to N_a. The flux Φ piercing the ring is produced by a solenoid inserted inside the ring.

$$(E+2\cos(K_1+\alpha)+2\cos(K_2+\alpha))f_{K_1,K_2} = \frac{U}{N_a}\sum_K f_{K_1-K,K_2+K}, \tag{4}$$

where $K_{1,2}=(2\pi/N_a)n_{1,2}$ with $n_{1,2}=0,1,2,\ldots,N_a-1$. Here f_{K_1,K_2} is assumed to satisfy the periodicity condition $f_{K_1+2\pi,K_2}=f_{K_1,K_2+2\pi}=f_{K_1,K_2}$. Equation (4) can be rewritten as follows:

$$P_Q\left(1-\frac{U}{N_a}\times\sum_p \frac{1}{E+2\cos(K_1-p+\alpha)+2\cos(K_2+p+\alpha)}\right)=0, \tag{5}$$

where $P_Q=(1/N_a)\Sigma_K f_{K_1-K,K_2+K}$, $Q=K_1+K_2=(2\pi/N_a)n$, and $p=(2\pi/N_a)m$. Hence, either the term inside the parentheses or P_Q should be equal to zero.

(I) $P_Q\neq 0$. **The Lieb and Wu solution**

For $P_Q\neq 0$, the term inside the parentheses should be equal to zero, or

$$\frac{1}{U}=S(E), \tag{6}$$

where

$$S(E)=\frac{1}{N_a}\sum_p \frac{1}{E+2\cos(K_1-p+\alpha)+2\cos(K_2+p+\alpha)}. \tag{7}$$

Using the Poisson summation formula,

$$\frac{1}{U}=\sum_{n=-\infty}^{\infty}\int_0^{2\pi}\frac{dp}{2\pi}\frac{\exp(ipN_an)}{E+4\cos(Q/2-p)\cos(Q/2+\alpha)} \tag{8}$$

$S(E)$ becomes

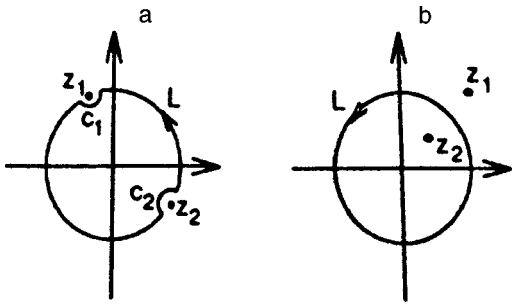

FIG. 2. Poles of the integrand in the complex plane. $E^2<E_0^2$ (a) and $E^2>E_0^2$ (b), where $E_0=-4\cos\beta$ for even n and $E_0=-4\cos\beta\cos(\pi/N_a)$ for odd n.

$$S(E)=\sum_{n=-\infty}^{\infty}S_n(E)\equiv S_{n=0}(E)+\sum_{n=1}^{\infty}[S_n(E)+S_n^*(E)]. \tag{9}$$

$S_n(E)$ can be calculated by transforming Eq. (8) to an integral in the complex plane. Setting $z=e^{ip}$, we have

$$S_n(E)=\frac{1}{2\pi i}\times\oint dz\,\frac{z^{N_an}}{z^2(e^{i\alpha}+e^{-i(Q+\alpha)})+Ez+(e^{i(Q+\alpha)}+e^{-i\alpha})}. \tag{10}$$

The poles (Fig. 2) of the integrand are

$$z_{1,2}=-\frac{-E\pm(E^2-E_0^2)^{1/2}}{E_0\exp(-iQ/2)}, \tag{11}$$

where $E_0=4\cos(Q/2+\alpha)$. For $E^2<E_0^2$, both of the poles z_1 and z_2 are on the unit circle and $S_{n=0}$ vanishes, while for $E^2>E_0^2$ one of them is inside the unit circle and the other one is outside of it, and $S_{n=0}$ does not vanish. For both cases

$$S(E)=\frac{1}{4i\sin x\cos\beta}\frac{\exp(i(Q/2-x)N_a)+1}{\exp(i(Q/2-x)N_a)-1}, \tag{12}$$

where x can be real or complex, depending on whether E^2 is smaller or larger than E_0^2, and $\beta=Q/2+\alpha$. If we denote new momenta k_1,k_2 as

$$k_{1,2}=\frac{Q}{2}+\alpha\pm x, \tag{13}$$

Eq. (6) takes the form

$$\exp[i(k_{1,2}-\alpha)N_a]=\frac{\sin k_{1,2}-\Lambda+iU/4}{\sin k_{1,2}-\Lambda-iU/4}, \tag{14}$$

where

$$\Lambda=\frac{\sin k_1+\sin k_2}{2}. \tag{15}$$

Equation (14) is identical to the Lieb and Wu solution[9] in the $\alpha=0$ limit.

It is possible to express the eigenvalue E of the system as

TABLE I. Minimum energy for different values of U.

	$U>0$	$U<0$	
even n	$E=-4\cos x\cos\beta$ with x (real) determined by $\tan(N_a x/2)=U/4\sin x\cos\beta$	$E=-4\cosh\kappa\cos\beta$ with κ determined by $\tanh(N_a\kappa/2)=\lvert U\rvert/4\sinh\kappa\cos\beta$	
		$U<U_{cr}$	$U_{cr}<U<0$
odd n	$E=-4\cos\beta\cos(\pi/N_a)$	$E=-4\cosh\kappa\cos\beta$, where κ is determined by $\tanh(N_a\kappa/2)=4\sinh\kappa\cos\beta/\lvert U\rvert$	$E=-4\cos x\cos\beta$, where x is determined by $\tan(N_a\kappa/2)=4\sinh x\cos\beta/\lvert U\rvert$

$$E=-2(\cos k_1+\cos k_2)=-4\cos x\cos\beta, \tag{16}$$

with x determined by

$$\tan\frac{N_a x}{2}=-\sigma\left(\frac{4\sin x\cos\beta}{U}\right)^{\sigma}, \tag{17}$$

where $\sigma=+1$ or -1 for odd or even value of $n[n=Q/(2\pi/N_a)]$.

For $U>0$, E^2 is always less than E_0^2; hence x is always real. For $U<0$ with even n, E^2 is always larger than E_0^2, so that x is complex. But for odd n and small $|U|$ values ($U<0$), x might be real. Let us consider Eq. (17) for negative U and odd n with complex $x=i\kappa$

$$\frac{1}{|U|}=\frac{\tanh(N_a\kappa/2)}{4\sinh\kappa\cos\beta}. \tag{18}$$

To have a solution of this equation, $1/|U|$ should not be larger than the maximum value of its right-hand side. Accordingly, the critical value $|U_{cr}(N_a)|$ can be found. The values of $|U|$ which are smaller than this $|U_{cr}|$ have real x; others have complex x in Eq. (17).

(II) $P_Q=0$. **The new state**

If P_Q is equal to zero, then either a new eigenvalue of the system is found as

$$E=-2\cos(q+\alpha)-2\cos(Q-q+\alpha), \tag{19}$$

with $K_1=q$ and $K_2=Q-q$, or $f_{K_1K_2}=0$ for any K_1 and K_2. But all f's cannot be zero; otherwise $|\Psi\rangle=0$. Summation of all f's, so that P_Q is equal to zero while f's are individually not all zero only if for two different values of q, $2\cos(q+\alpha)+2\cos(Q-q+\alpha)$ are coinciding.

For positive on-site interaction U, this eigenvalue becomes the minimum energy of the system when n is odd. For $U<0$ it does not become the minimum eigenvalue of the system.

The ground-state energy values are summarized in Table I.

The dependence of the ground-state energy on the flux is shown in Fig. 3.

A. Dependence of the amplitude of energy oscillations on the number of sites

The dependence $E(\Phi)$ is shown schematically in Fig. 4, where ΔE_1 and ΔE_2 are the amplitudes of hc/e and $hc/2e$ oscillations.

For $U<U_{cr}<0$ in the large N_a limit

$$\Delta E_1=\Delta E_2=\Delta E\approx\frac{2\pi^2}{N_a^2}\frac{1}{(U^2+16)^{1/2}}. \tag{20}$$

Here there is a $\Phi_0/2$ periodicity, which resembles the pairing of electrons as in a superconductor, but the amplitude of the energy oscillations decreases with inverse square of the

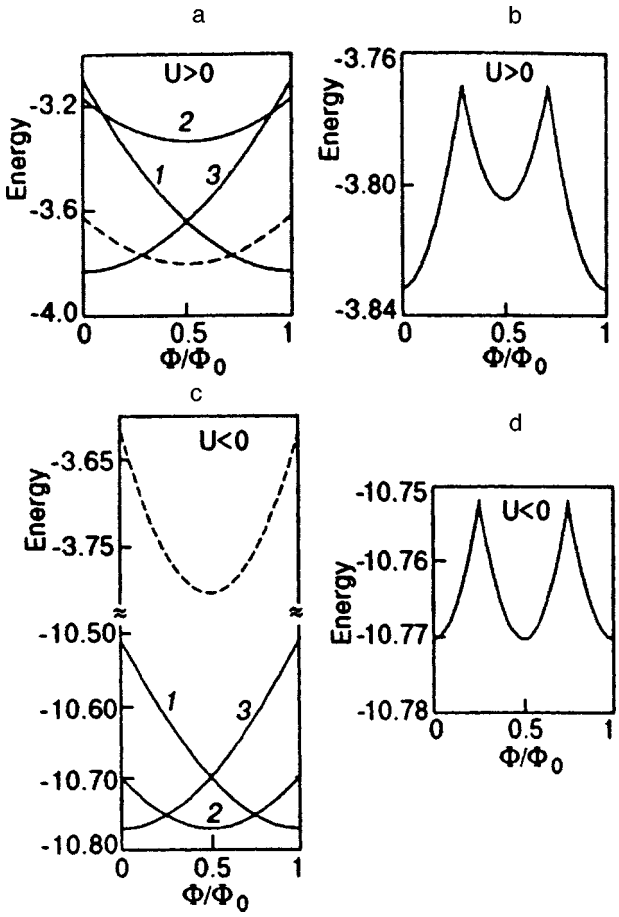

FIG. 3. Energy versus flux for two electrons with $N_a=10$. (a) Solid curves *1–3* correspond to the Lieb–Wu solution and the dashed curve corresponds to the new states found by us. For $U>0$ ($U=10$) this new state becomes the minimum energy of the system. (b) The same as (a) to show the $\Phi_0/2$ periodicity more clearly. It is clearly seen that the Lieb–Wu solution (solid curves *1–3*) does not lead to the $\Phi_0/2$ periodicity alone. (c) $U=-10$. As in (a), the solid curves *1–3* are the lowest-lying eigenvalues found by the Lieb–Wu solution. Similarly, the dashed curve corresponds to the new state found by us. For $U<0$ the new eigenvalue does not become the minimum energy of the system. (d) The same as (c) to show the periodicity more clearly.

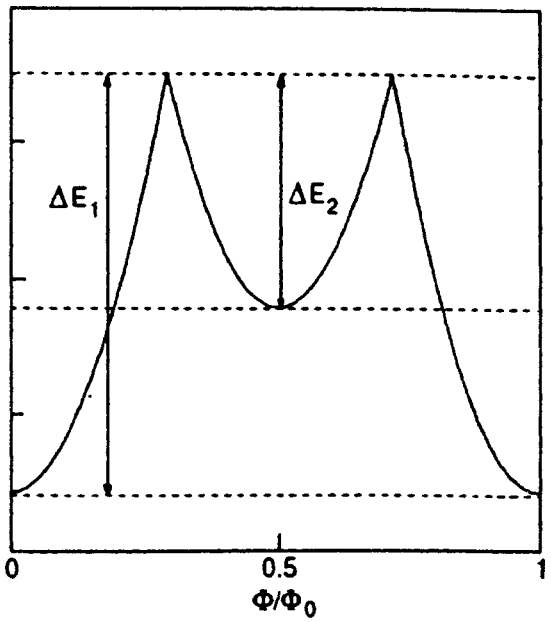

FIG. 4. Energy oscillations for two electrons. ΔE_1—amplitude of hc/e periodicity, ΔE_2—amplitude of $hc/2e$ periodicity.

number of lattice sites (Fig. 5a). If $|U|\to|U_{cr}|$, then the amplitude of oscillation corresponding to $hc/2e$ becomes smaller and at $U=U_{cr}$ it vanishes. Note, however, that for very large values of N_a, $|U_{cr}|$ becomes quite small; hence even for very small $|U|$ the behavior of energy with respect to flux is the same. The behavior of ground-state energy is shown explicitly for various values of U and N_a in Figs. 5c–5f. In the very large N_a limit, using Eqs. (16) and (17), we can show that

$$E\approx-\sqrt{U^2+16\cos^2\beta} \tag{21}$$

for even and odd values of n. The last expression can be obtained directly from Eq. (7) by changing the summation over p to an integral.

For $U>0$, in the limit $N_a\gg1$

$$\Delta E_1\approx\frac{2\pi^2}{N_a^2}\left(1-\frac{1}{2}\left(\frac{UN_a}{8+UN_a}\right)^2\right)^2, \tag{22}$$

$$\Delta E_2\approx\frac{2\pi^2}{N_a^2}\left(\frac{1}{2}\left(\frac{UN_a}{8+UN_a}\right)^2\right)^2. \tag{23}$$

Hence, for $U\times N_a\to\infty$, $\Delta E_1=\Delta E_2=1/4(2\pi^2/N_a^2)$. Both ΔE_1 and ΔE_2 behave like $1/N_a^2$, and $\Delta E_1/\Delta E_2\to1$ (Fig.

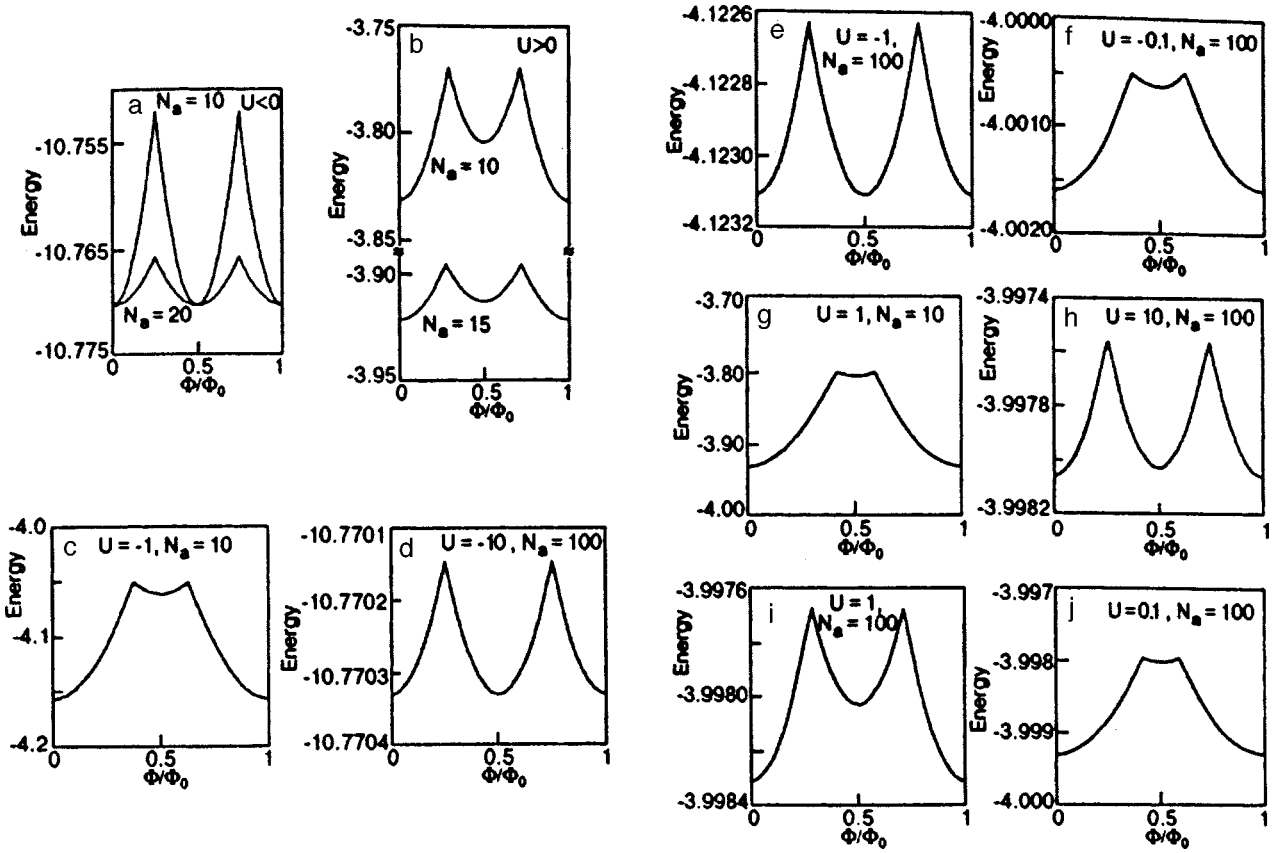

FIG. 5. (a) Minimal energy versus flux for $N_a=10$ and 20 ($U=-10$). Comparison of oscillations for $N_a=10$ and 20 shows the $1/N_a^2$ behavior of the amplitude. (b) Minimal energy versus flux for $N_a=10$ and 15 ($U=10$). As the number of sites increases (larger N_a), $\Delta E_1/\Delta E_2$ approaches 1. (c–f) Ground-state energy for different values of N_a and negative U. Compared to the oscillations in (a) for $N_a=10$ amplitude ΔE_2 becomes smaller in (c). This occurs because U comes closer to U_{cr}, if larger values of U were used, even smaller ΔE_2 values would be obtained. (d), (e), and (f) demonstrates the behavior of the system with $N_a=100$. This time even with $U=-1$, ΔE_2 is still almost equal to ΔE_1, because for larger values of N_a, U_{cr} becomes larger and approaches zero. For $U=-0.1$ a decrease in ΔE_2 is observed. (g–j) Ground-state energy for different values of N_a and for positive U. For smaller values of $U(U\to0)\Delta E_2$ becomes smaller. But just as in the $U<0$ case, for larger values of N_a, even for very small values of U, there is still a $\Phi_0/2$ periodicity. It should be noted that in all cases, as $N_a\to\infty$, all oscillations vanish, $\Delta E_{1,2}\to0$.

5b). But for $U\to 0$, $U\times N_a\to 0$; $\Delta E_1=2\pi^2/N_a^2$ and $\Delta E_2=0$. The plots of energy versus flux behavior of the system for positive U are shown explicitly in Figs. 5g–5j.

With the new state found in our work, an $hc/2e$ periodicity of the ground-state energy appears even for positive U. This branch vanishes gradually as $U\to 0$. It is not possible to find this periodicity with the Lieb–Wu solution.

B. Comparison with other theories

The energy oscillations with the $hc/2e$ periodicity were calculated in the strongly correlated electron models, including the Hubbard model, in a number of papers.[11–17] In some papers[18–21] the Hubbard model was examined by using the Lieb and Wu solution.[9] The oscillations with the $hc/2e$ periodicity for negative U can be found by starting directly from the original solution presented by Lieb and Wu, since the new state found in our work does not become the minimum energy state. But for positive U, new states should be included to obtain the correct $hc/2e$ periodicity. The Lieb and Wu solution does not lead to the $hc/2e$ periodicity for positive U.

1) Why Lieb–Wu is incomplete:
Let us consider the Lieb–Wu equations (with no magnetic flux Φ)

$$\exp(iN_ak_1)=\frac{\sin k_1-\sin k_2+iU/2}{\sin k_1-\sin k_2-iU/2}, \tag{24}$$

$$\exp(iN_ak_2)=\frac{\sin k_2-\sin k_1+iU/2}{\sin k_2-\sin k_1-iU/2}. \tag{25}$$

Dividing the first equation by the second, with $k_1+k_2=Q$ and $k_1-k_2=2\kappa$, we obtain

$$\exp(2iN_a\kappa)=\left(\frac{2\sin\kappa\cos(Q/2+\alpha)+iU/2}{2\sin\kappa\cos(Q/2+\alpha)-iU/2}\right)^2. \tag{26}$$

The energy equation is

$$E=-2(\cos k_1+\cos k_2)=-4\cos(Q/2)\cos\kappa, \tag{27}$$

and the new eigenvalue found by us is

$$E=-4\cos(Q/2)\cos(\pi/N_a). \tag{28}$$

Therefore, κ should be equal to π/N_a in Eq. (27). According to Eq. (26) it is obvious that this is possible only if $U=0$. The Lieb–Wu solution does not give this result for all U except $U=0$.

In the original paper of Lieb and Wu[9] it is explicitly stated that the momenta k_j should be unequal, which means that both I_1-I_2 and I_1+I_2 cannot be equal to zero (I_1 and I_2 are integers in the original paper of Lieb and Wu.[9] This is also the case in our procedures. In terms of our approach, $\kappa=0$ should be excluded from the solution set. But in some papers[14] k_1 is assumed to be equal to k_2, so that $\kappa=0$ and a $\Phi_0/2$ periodicity is obtained by accident.

3. CONTRACTION MODEL

A. Physical background

In the investigation of unusual electronic properties of metal-oxide compounds it was proposed[7,8,22] that the new features in the electronic band conduction in oxide metals should be included. The first one is the possibility that ''intrinsic-hole'' rather than intrinsic-electron carriers may play a role. The second one is that, provided intrinsic holes are at work, one-particle picture of the electronic transport is not fully adequate, because the interaction between holes (repulsive or attractive) must be included, and because the fact that the hopping of holes in itself cannot be considered as constant in amplitude and is strongly dependent upon site occupation.

Normally, two oxygen atoms have a strong tendency to make covalent bonding, which results in the formation of an oxygen molecule, O_2. However, in a proper chemical surrounding, this may not happen if the nearest neighbor atoms are not too close to each other. In this case the other scenario, which is reminiscent of metallic oxygen, applies. We can assume that this is just what happens in the metal-oxide superconductors. In the CuO_2 plane of the latter, due to large ionic radii of oxygen, the oxygen orbitals overlap each other almost as strongly as the near site oxygen and copper orbitals do. The O_2 molecules therefore are not formed, and the electrons derived from the p^6 shell are the conducting electrons. The charge carriers are holes in the p^6 shell, which propagate from one oxygen anion to the next nearest one by hopping. Because of the contraction of the p orbital of oxygen as a result of occupation by a hole, hole hopping between nearest-neighbor sites (i,j) is dependent on the opposite-spin hole occupation number. In the second quantization representation it was suggested to consider the hopping matrix element t_{ij} as an operator which depends on the occupation number operators n_i and n_j at the atomic sites R_i and R_j. There are three independent matrix elements, t_0, t_1, and t_2 (Refs. 23 and 26), which in the case of two oxygen anions correspond to the following, charge transfer reactions:

$$\begin{aligned} t_0&:\quad \mathrm{O}_i^-+\mathrm{O}_j^{2-}\to\mathrm{O}_i^{2-}+\mathrm{O}_j^-\\ t_1&:\quad \mathrm{O}_i+\mathrm{O}_j^{2-}\to\mathrm{O}_i^{2-}+\mathrm{O}_j,\\ t_2&;\quad \mathrm{O}_i+\mathrm{O}_j^-\to\mathrm{O}_i^-+\mathrm{O}_j, \end{aligned} \tag{29}$$

which result in

$$\begin{aligned} t_{ij}=t_0(1-n_{i,-\sigma})(1-n_{j,-\sigma})+t_1[n_{i,-\sigma}(1-n_{j,-\sigma})\\ +n_{j,-\sigma}(1-n_{i,-\sigma})]+t_2n_{i,-\sigma}n_{j,-\sigma}. \end{aligned} \tag{30}$$

The occupation dependence of the hopping can be represented in another form:

$$t_{ij}=-t+Vn_{i,-\sigma}n_{j,-\sigma}+W(n_{i,-\sigma}+n_{j,-\sigma}), \tag{31}$$

where from Eq. (30) we obtain

$$t=-t_0,\quad V=t_0-2t_1+t_2,\quad W=t_1-t_0. \tag{32}$$

Hence, the $1D$ version of the interacting holes in an anion network can be represented by the following Hamiltonian, which includes the on-site interaction term U:

$$H=-\sum_{j\sigma} c_{j\sigma}^{+}c_{j+1,\sigma}\exp(i\alpha)+\text{H.c.}+U\sum_{j} n_{j\uparrow}n_{j\downarrow}$$
$$+\sum_{j,\sigma} c_{j\sigma}^{+}c_{j+1,\sigma}[Vn_{j,-\sigma}n_{j+1,-\sigma}+W(n_{j,-\sigma}$$
$$+n_{j+1,-\sigma})]\exp(i\alpha)+\text{H.c.} \tag{33}$$

The effect of the coupling term W has been considered in great detail in the paper of Hirsch and Marsiglio,[7] as well as by Kulik *et al.*[8,25]

B. Bound state of two electrons

As before, we use the wave function for two electrons, one with spin up and the other with spin down,

$$|\Psi\rangle=\sum_{x_1,x_2} f(x_1,x_2)c_{x_1\downarrow}^{+}c_{x_2\uparrow}^{+}|0\rangle. \tag{34}$$

In momentum space the eigenvalue equation $H|\Psi\rangle=E|\Psi\rangle$ gives

$$\begin{bmatrix} 1-US_0(E)-WS_1(E) & -WS_0(E) \\ US_1(E)+WS_2(E) & -1+WS_1(E) \end{bmatrix}\times\begin{bmatrix} F_0(Q) \\ F_1(Q) \end{bmatrix}=0, \tag{35}$$

where

$$\frac{1}{N_a}\sum_{K}(\varepsilon_{K_1-K+\alpha}+\varepsilon_{K_2+K+\alpha})^{n}f_{K_1-K,K_2+K}\equiv F_n(Q), \tag{36}$$

$n=0$, 1, and

$$\frac{1}{N_a}\sum_{p}\frac{(\varepsilon_{K_1-p+\alpha}+\varepsilon_{K_2+p+\alpha})^{n}}{E+(\varepsilon_{K_1-p+\alpha}+\varepsilon_{K_2+p+\alpha})}\equiv S_n(E), \tag{37}$$

$n=0$, 1, 2; $\varepsilon_k=2\cos k$. Hence, either the determinant of the first matrix is equal to zero or both terms of the vector are zero.

For two electrons V does not show up. The effect of V in the weak-coupling regime was considered previously.[8]

In the case $F_0=F_1=0$ the energy eigenvalue of the system becomes

$$E=-2\cos(q+\alpha)-2\cos(Q-q+\alpha)$$
$$=-4\cos(Q/2-q)\cos\beta. \tag{38}$$

It is possible to have both F_0 and F_1 equal to zero, while all f's are not individually equal to zero only if for two different values of q, $2\cos(q+\alpha)+2\cos(Q-q+\alpha)$ are coinciding.

For the other case, i.e., when determinant of the first matrix in Eq. (35) is equal to zero, the transcendental equation is found as follows:

$$\frac{(W-1)^2}{U+W(W-2)E}=S_0(E). \tag{39}$$

The plot of $S_0(E)$ is presented in Fig. 6. Equation (39) can be solved numerically, which is done to test our results. If we set $W=0$ in the last equation, we immediately obtain the result of the $1D$ Hubbard model discussed in Sec. 2. With similar calculations as in the previous sections, the minimum energy corresponding to Eq. (39) is found as

$$E=-(\cos k_1+\cos k_2)=-4\cos x\cos\beta, \tag{40}$$

where x is determined by

$$\tan\frac{N_a x}{2}=-\sigma\left(\frac{4(W-1)^2\sin x\cos\beta}{U-4W(W-2)\cos x\cos\beta}\right)^{\sigma}. \tag{41}$$

Here $\sigma=+1$ or -1 for odd or even values of n. In the hatched region in Fig. 7 for odd values of n the expression

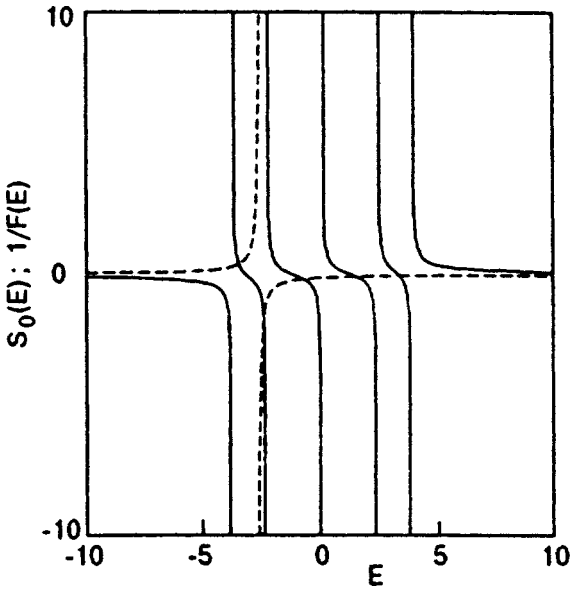

FIG. 6. Plot of the transcendental equation for the contraction model. The intersection points of $S_0(E)$ (solid line) with $1/F(E)$ (dashed line) give the energy eigenvalues. Here $N_a=10$, $\Phi=\Phi_0/2$, $n=9$, $U=-2$, and $W=1.5$.

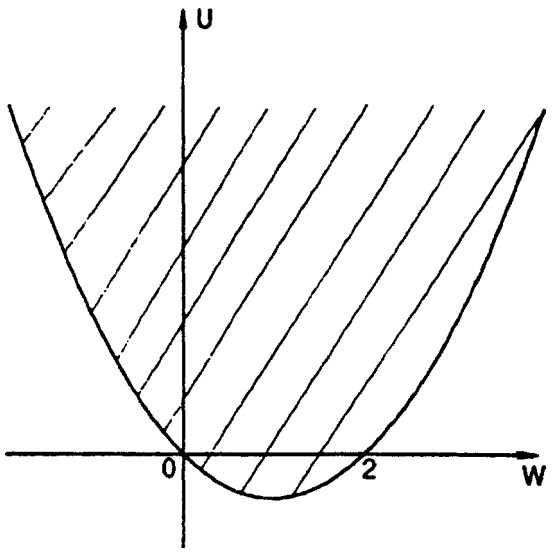

FIG. 7. Phase space for bound states of two electrons. The hatched region corresponds to the free propagating states and the nonhatched region corresponds to the bound states of two electrons within the contraction model. The solid line corresponds to the equation $U=-W(W-2)E_1$, where $E_1=-4\cos\beta$ for even n and $E_1=-4\cos\beta\cos(\pi/N_a)$ for odd n.

TABLE II. Minimum energy for different values of U.

	$U>-W(W-2)E_1$ hatched part in Fig. 7	$U<-W(W-2)E_1$ nonhatched part in Fig. 7	
even n	$E=-4\cos x\cos\beta$ with x (real) determined by $\tan\left(\frac{N_a x}{2}\right)=\frac{U-4W(W-2)\cos x\cos\beta}{4(W-1)^2\sin x\cos\beta}$	$E=-4\cosh\kappa\cos\beta$ with κ (real) determined by $\tanh\frac{N_a\kappa}{2}=-\frac{U-4W(W-2)\cosh\kappa\cos\beta}{4(W-1)^2\sinh\kappa\cos\beta}$	
		$U<U_{cr}$	$U>U_{cr}$
odd n	$E=-4\cos\beta\cos(\pi/N_a)$	$E=-4\cosh\kappa\cos\beta$, where κ is determined by $\tanh\frac{N_a\kappa}{2}=-\frac{4(W-1)^2\sinh\kappa\cos\beta}{U-4W(W-2)\cosh\kappa\cos\beta}$	$E=-4\cos x\cos\beta$, where x is determined by $\tan\frac{N_a x}{2}=-\frac{4(W-1)^2\sin x\cos\beta}{U-4W(W-2)\cos x\cos\beta}$

$$E=-4\cos(\pi/N_a)\cos\beta \tag{42}$$

gives the minimum energy value. The curve in Fig. 7 corresponds to $U=-W(W-2)E_1$, where $E_1=-4\cos\beta$ for even n and $E_1=-4\cos\beta\cos(\pi/N_a)$ for odd n. The resulting values of the ground-state energy for different values of U and W are summarized in Table II.

Here U_{cr} is found in a similar way to that of the Hubbard model. The energy-versus-flux dependence for two electrons in the contraction model is shown in Fig. 8.

The amplitudes of the energy oscillations in the $N_a\gg 1$ limit are found as follows:

(i) For the nonhatched region below the curve (the bound states) and $U<U_{cr}$ ($U<U_{cr}<-W(W-2)E_1$):

$$\Delta E_1=\Delta E_2=\Delta E$$

$$\approx\frac{(2\pi^2/N_a^2)(W-1)^4}{\{U^2W^2(W-2)^2+(2W^2-4W+1)[16(W-1)^4+U^2]\}^{1/2}}. \tag{43}$$

Hence there is a $\Phi_0/2$ periodicity. The branch corresponding to the expression in Eq. (42) for odd n does not become the minimum energy; it is shown as a dashed line in Fig. 8a. As $U\to U_{cr}$ from below, the branch which is marked as 2 in Fig. 8c fades away from being the minimum energy. Eventually, at $U=U_{cr}$ there is no more $\Phi_0/2$ periodicity. For very large $N_a(N_a\to\infty)$, $U_{cr}\to 4W(W-2)$. It is interesting that in this very large N_a limit $E_1\to -4$, so that the curve in Fig. 7 corresponds to $U=4W(W-2)\sim U_{cr}$. Hence, for very large N_a, any U which satisfies $U<4W(W-2)$ is less than U_{cr}; therefore, almost always there is a $\Phi_0/2$ periodicity in the nonhatched region in Fig. 7.

(ii) For the shaded region above the curve in Fig. 7 the expression in Eq. (42) becomes the minimum energy of the system. This branch is shown as the dashed line in Fig. 8a. The corresponding amplitudes are

$$\Delta E_1\approx(2\pi^2/N_a^2)(1-\lambda)^2, \tag{44}$$

$$\Delta E_2\approx(2\pi^2/N_a^2)\lambda^2, \tag{45}$$

where

$$\lambda=\frac{1}{2}\left(\frac{(U-4W(W-2))N_a}{8(W-1)^2+N_a[U-4W(W-2)]}\right)^2. \tag{46}$$

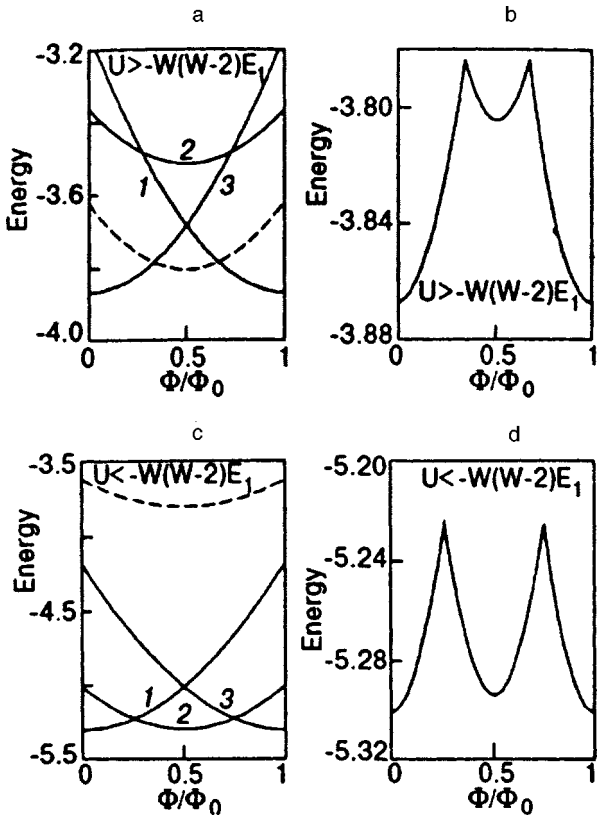

FIG. 8. Energy versus flux for two electrons in the contraction mechanism. Note the resemblance of this figure to Fig. 3. Here instead of $U>0$ there is $U>-W(W-2)E_1$; similarly for $U<0$ there is the $U<-4W(W-2)$ criterion. In (a) the solid curves correspond to the expression (40) and the dashed curve corresponds to the expression (42). Just like for $U>0$ in the Hubbard model, in the contraction model for $U>-W(W-2)E_1$ the dashed curve becomes the minimal energy of the model. (b) The same as (a) to show the behavior of the system more clearly. In (a) and (b) $N_a=10$, $U=-2$, $W=1.5$. In (c) $U<-W(W-2)E_1$, just as in the Hubbard model for $U<0$, the solution corresponding to Eq. (42) does not take place as the minimum energy of the model. The solid curves *1–3* correspond to Eq. (40) and the dashed curve corresponds to Eq. (42). (d) is the same as (c) to show the behavior more clearly. In (c) and (d) $N_a=10$, $U=2$, and $W=-1$.

For $(U-4W(W-2))N_a \to \infty$, $\Delta E_1 = \Delta E_2 = 1/4(2\pi^2/N_a^2)$. But for $(U-4W(W-2))N_a \to 0$, $\Delta E_1 = 2\pi^2/N_a^2$, and $\Delta E_2 = 0$.

All results found here and in the previous section for the Hubbard model are in close correlation. In the Hubbard model and the contraction model two different types of solutions were found. For the Hubbard model a new type of solution gives the $\Phi_0/2$ periodicity for $U>0$, which is absent in the Lieb–Wu solution, while in the contraction model this type of solution gives the $\Phi_0/2$ periodicity for $U>-W(W-2)E_1$. In the Hubbard model for $U<0$ can be larger or smaller than E_0, depending on whether U is larger or smaller than a critical value U_{cr}. Similarly for the contraction model for $U<-W(W-2)E_1, E$ can be larger or smaller than E_0, depending on whether U is larger or smaller than U_{cr}. For Hubbard model U_{cr} becomes zero for very large N_a, for contraction model it becomes $4W(W-2)$. In all these inequalities one can get Hubbard model type relations setting $W=0$ in contraction model relations.

4. CONCLUSIONS

In the one-dimensional Hubbard model and the contraction model for two electrons, the periodicity of ground-state energy with respect to flux is $hc/2e$. Our study shows that the solution for a one-dimensional Hubbard model by Lieb and Wu[9] in 1968 is not complete, at least for two electrons. For positive on-site interaction new states found by us correspond to the ground-state energy. Hence, they play an important role for correct behavior of the ground-state energy of the system. Generalizing the current results to more than two electrons will be the task of a future work. It is very likely that for more than two electrons new states, which cannot be determined by the Lieb and Wu results, will be found. The model for the ground-state energy of contraction has a $hc/2e$ periodicity also. But it is not easy to speak about superconductivity very clearly. For some range of the values of U and W it is likely that this model results in superconductivity. To show that this model serves as a model for superconductivity, other probing methods should be used.

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